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货币族金属化合物的结构和光学性能研究

Structure and Optical Properties of Coinage

Metal Complexes

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# **Structure and Optical Properties of Coinage Metal Complexes**

A Dissertation Submitted to the Graduates School in Partial Fulfillment of  
the Requirements for the Degree of Doctor Philosophy

By

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## 论文用词简写

简写	名称或分子式
bdt	1,2-benzenedithiol
BPA	HN(CH <sub>2</sub> -2-C <sub>5</sub> H <sub>4</sub> N <sub>2</sub> )
bzim	1-benzyl-2-imidazolate
carb	-C(OEt)=NC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> -p
cdpp	bis(diphenylphosphine)vinylidene
dbfphos	4,6-bis(diphenylphosphino)dibenzofuran
dcpe	1,2-bis(dicyclohexylphosphino)ethane
dcpm	bis(dicyclohexylphosphino)methane
DMSO	dimethylsulfoxide
dpephos	bis[(2-diphenylphosphino)phenyl]ether
dpepp	bis(2-diphenylphosphinoethyl)phenylphosphine
dppa	1,2-bis(diphenylphosphino)acetylene
dppb	1,4-bis(diphenylphosphino)butane
dppbe	1,2-bis(diphenylphosphino)benzene
dppbp	4,4'-bis(diphenylphosphino)biphenyl
dppe	1,2-bis(diphenylphosphino)ethane
dppf	1,1-bis(diphenylphosphino)ferrocene
dpph	1,6-bis(diphenylphosphino)hexane
dppp	1,3-bis(diphenylphosphino)propane
dpppe	1,5-bis(diphenylphosphino)pentane
dppm	bis(diphenylphosphino)methane
dppy	diphenyl-2-pyridylphosphine
IL	intraligand
im	imidazol
L	ligand
LMCT	ligand to metal charge transfer
M	metal
MC	metal-centered
mes	mesityl

MLCT	metal to ligand charge transfer
NSLF	non-linear least square fit
OLED	organic light emitting diode
OTf	trifluoromethylsulfonate
<i>P</i>	monodentate phosphine
<i>P~P</i>	bidentate phosphine
<i>P~P~P</i>	tridentate phosphine
py	pyridine
3,5-Ph <sub>2</sub> pz	3,5-diphenylpyrazole
SeU	selenourea
THF	tetrahydrofuran
tht	tetrahydrothiophene
tmeda	N,N,N',N'-tetramethylenediamine
TPA	1,3,5-triaza-7-phosphaadamantane
Tab	4-(trimethylammonio)benzenethiolate
tacn	1,4,7-triazacyclononane
terpy	2,2':6',2''-terpyridine
Tfa	trifluoroacetate
Tol	tolyl
tpep	1,1,1-tris(diphenylphosphinoethyl)phosphine
tpep <sup>Se</sup>	1,1,1-bis(diphenylphosphinoethyl)-1-(diphenylseleno phosphinoethyl)phosphine
VOCs	volatile organic compounds
VSEPR	valence shell electron pair repulsion
X	halogen
xantphos	9,9-dimethyl-4,5-bis(diphenylphosphino)xanthene

## 化合物索引

序号	简写	名称或分子式
1	<b>L1</b>	diphenyl-2-pyridylphosphine
2	<b>L2</b>	2-diphenylphosphino-3-methylpyridine
3	<b>L3</b>	2-diphenylphosphino-4-methylpyridine
4	<b>L4</b>	2-diphenylphosphino-5-methylpyridine
5	<b>L5</b>	2-diphenylphosphino-6-methylpyridine
6	<b>L6</b>	2-diphenylphosphino-6-methoxypyridine
7	<b>A1</b>	$[\text{CAu}_6(\text{L1})_6](\text{BF}_4)_2$
8	<b>A2</b>	$[\text{CAu}_6(\text{L2})_6](\text{BF}_4)_2$
9	<b>A3</b>	$[\text{CAu}_6(\text{L3})_6](\text{BF}_4)_2$
10	<b>A4</b>	$[\text{CAu}_6(\text{L4})_6](\text{BF}_4)_2$
11	<b>A5</b>	$[\text{CAu}_6(\text{L5})_6](\text{BF}_4)_2$
12	<b>A6</b>	$[\text{CAu}_6(\text{L6})_6](\text{BF}_4)_2$
13	<b>A7</b>	$[\text{CAu}_6\text{Ag}_2(\text{L1})_6](\text{BF}_4)_4$
14	<b>A8</b>	$[\text{CAu}_6\text{Ag}_2(\text{L2})_6](\text{BF}_4)_4$
15	<b>A9</b>	$[\text{CAu}_6\text{Ag}_2(\text{L3})_6](\text{BF}_4)_4$
16	<b>A10</b>	$[\text{CAu}_6\text{Ag}_2(\text{L4})_6](\text{BF}_4)_4$
17	<b>A11</b>	$[\text{CAu}_6\text{Ag}_2(\text{L6})_6](\text{BF}_4)_4$
18	<b>A12</b>	$[\text{CAu}_6\text{Ag}_2(\text{L6})_4(\text{L2})_2](\text{BF}_4)_4$
19	<b>A13</b>	$[\text{CAu}_6\text{Cu}_2(\text{L1})_6](\text{BF}_4)_4$
20	<b>A14</b>	$[\text{CAu}_6\text{Cu}_2(\text{L2})_6](\text{BF}_4)_4$
21	<b>A15</b>	$[\text{CAu}_6\text{Cu}_2(\text{L3})_6](\text{BF}_4)_4$
22	<b>A16</b>	$[\text{CAu}_6\text{Cu}_2(\text{L4})_6](\text{BF}_4)_4$
23	<b>A17</b>	$[\text{CAu}_6\text{Ag}_3(\text{L5})_6](\text{BF}_4)_5$
24	<b>A18</b>	$[\text{CAu}_6\text{Cu}_3(\text{L5})_6](\text{BF}_4)_5$
25	<b>A19</b>	$[\text{CAu}_6\text{AgCu}(\text{L1})_6](\text{BF}_4)_4$
26	<b>A20</b>	$[\text{CAu}_6(\text{PPh}_3)_6](\text{BF}_4)_2$
27	<b>B1</b>	$[\text{Au}_4(\mu_2\text{-S})_2(\mu\text{-dppb})_2]$
28	<b>B2</b>	$[\text{Au}_4(\mu_2\text{-S})_2(\mu\text{-dppp})_2]$
29	<b>B3</b>	$[\text{Au}_5(\mu_3\text{-S})_2(\mu\text{-dppp})_2]\text{Cl}$

30	<b>B4</b>	$[\text{Au}_5(\mu_3\text{-S})_2(\mu\text{-dppp})_2](\text{BF}_4)$
31	<b>B5</b>	$[\text{Au}_5(\mu_3\text{-S})_2(\mu\text{-dppp})_2](\text{Tfa})$
32	<b>B6</b>	$[\text{Au}_5(\mu_3\text{-S})_2(\mu\text{-dppp})_2](\text{OTf})$
33	<b>B7</b>	$[\text{Au}_{10}(\mu_3\text{-S})_4(\mu\text{-dcpm})_4]\text{Cl}_2$
34	<b>B8</b>	$[\text{Au}_{10}(\mu_3\text{-S})_4(\mu\text{-dcpe})_4]\text{Cl}_2$
35	<b>B9</b>	$[\text{Au}_9(\text{AuCl})_2(\mu_3\text{-S})_4(\mu\text{-xantphos})_4]\text{Cl}$
36	<b>B10</b>	$[\text{Au}_{13}(\mu_3\text{-S})_6(\mu\text{-xantphos})_4]\text{Cl}$
37	<b>B11</b>	$[\text{Au}_{18}(\mu_3\text{-S})_8(\mu\text{-dppe})_6]\text{Cl}_2$
38	<b>B12</b>	$[\text{Au}_{18}(\mu_3\text{-S})_8(\mu\text{-dpephos})_6]\text{Cl}_2$
39	<b>B13</b>	$[\text{Au}_{12}(\mu_3\text{-S})_4(\mu\text{-dppm})_4]\text{Cl}_4$
40	<b>B14</b>	$[\text{Au}_{12}(\mu_3\text{-S})_4(\mu\text{-dppm})_4](\text{PF}_6)_4$
41	<b>B15</b>	$[\text{Au}_{10}(\mu_3\text{-S})_4(\mu\text{-PNP})_4](\text{PF}_6)_2$
42	<b>B16</b>	$[\text{Au}_{18}(\mu_3\text{-S})_8(\mu\text{-dppe})_6] \cdot \text{H}_2\text{O}$
43	<b>B17</b>	$[\text{Au}_6(\mu_3\text{-Se})_2(\mu_3\text{-dpepp})_2]\text{Cl}_2$
44	<b>B18</b>	$[\text{Au}_{14}(\mu_3\text{-Se})_6(\mu_3\text{-dppp})_5]\text{Cl}_2$
45	<b>B19</b>	$[\text{Au}_{18}(\mu_3\text{-Se})_8(\mu_3\text{-dppa})_6]\text{Cl}_2$
46	<b>B20</b>	$[(\text{AuPPh}_3)_3\text{Se}](\text{PF}_6)$
47	<b>B21</b>	$[(\text{AuPPh}_3)_4\text{Se}](\text{OTf})_2$
48	<b>B22</b>	$[\text{Au}_{10}\text{Se}_4(\text{dppm})_4]\text{Br}_2$
49	<b>B23</b>	$[\text{Au}_{18}\text{Se}_8(\text{dppe})_6]\text{Cl}_2$
50	<b>B24</b>	$[\text{Au}_{18}\text{Se}_8(\text{dpptph})_6]\text{Cl}_2$
51	<b>B25</b>	$[\text{Au}_{10}\text{Se}_5(\text{dppa})_4\{\text{Co}_2(\text{CO})_5\}_4]$
52	<b>B26</b>	$[\text{Au}_{10}\text{Se}_4(\text{dppf})_4](\text{NO}_3)_2$
53	<b>D1</b>	$[\text{Au}(\text{PPh}_3)(\text{PPT2})]$
54	<b>D2</b>	$[\text{Au}(\text{PPh}_3)(\text{PPT3})]$
55	<b>D3</b>	$[\text{Au}_2(\text{dppm})(\text{PPT2})_2] \cdot 0.5\text{CH}_2\text{Cl}_2$
56	<b>D4</b>	$[\text{Au}_2(\text{dppm})(\text{PPT4})_2] \cdot \text{CH}_3\text{COCH}_3$
57	<b>D5</b>	$[\text{Au}_2(\text{dppe})(\text{PPT2})_2]$
58	<b>D6</b>	$[\text{Au}_2(\text{dppe})(\text{PPT3})_2]$
59	<b>D7</b>	$[\text{Au}_2(\text{dppe})(\text{PPT4})_2]$
60	<b>D8</b>	$[\text{Au}_2(\text{dppp})(\text{PPT2})_2] \cdot 3\text{CH}_2\text{Cl}_2 \cdot \text{CH}_3\text{CH}_2\text{OH}$
61	<b>D9</b>	$[\text{Au}_2(\text{dppb})(\text{PPT2})_2]$
62	<b>D10</b>	$[\text{Au}_2(\text{dppb})(\text{PPT3})_2] \cdot 3\text{CH}_2\text{Cl}_2$



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